

STN Process Search - Cas react

10/537,389

07/20/2007,

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAJMN1626

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page for STN Seminar Schedule - N. America
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS 3 MAR 16 CASREACT coverage extended
NEWS 4 MAR 20 MARPAT now updated daily
NEWS 5 MAR 22 LWPI reloaded
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records
NEWS 10 APR 30 CA/Capplus enhanced with 1870-1889 U.S. patent records
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN
NEWS 12 MAY 01 New CAS web site launched
NEWS 13 MAY 08 CA/Capplus Indian patent publication number format defined
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields.
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload
NEWS 17 MAY 21 CA/Capplus enhanced with additional kind codes for German patents
NEWS 18 MAY 22 CA/Capplus enhanced with IPC reclassification in Japanese patents
NEWS 19 JUN 27 CA/Capplus enhanced with pre-1967 CAS Registry Numbers
NEWS 20 JUN 29 STN Viewer now available
NEWS 21 JUN 29 STN Express; Version 8.2, now available
NEWS 22 JUL 02 LEMBASE coverage updated
NEWS 23 JUL 02 LMEDLINE coverage updated
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names
NEWS 25 JUL 02 CHEMCATS accession numbers revised
NEWS 26 JUL 02 CA/Capplus enhanced with utility model patents from China
NEWS 27 JUL 16 Capplus enhanced with French and German abstracts
NEWS 28 JUL 18 CA/Capplus patent coverage enhanced

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
AND CURRENT DISCOVER FILE IS DATED 05 JULY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability

NEWS LOGIN Welcome Banner and News Items

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer

agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:00:56 ON 20 JUL 2007

=> fil casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'CASREACT' ENTERED AT 16:01:07 ON 20 JUL 2007

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 14 Jul 2007 VOL 147 ISS 4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

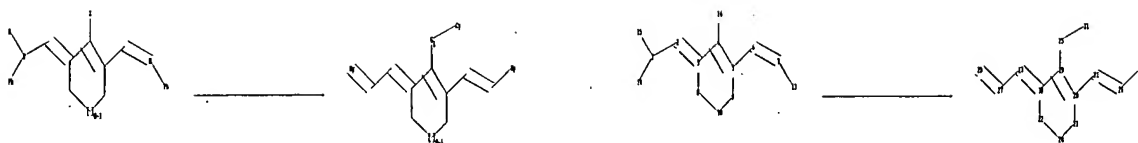
*
* CASREACT now has more than 12 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

Uploading C:\Program Files\Stnexp\Queries\10537389\1.str



chain nodes :

1 2 6 7 13 14 15 16 17 21 25 26 27 28 29 31

ring nodes :

3 4 5 8 9 10 18 19 20 22 23 24

chain bonds :

1-2 1-14 1-15 2-3 4-16 5-6 6-7 7-13 17-18 17-27 19-25 20-21 21-26
25-31 26-29 27-28

ring bonds :

3-4 3-8 4-5 5-9 8-10 9-10 18-19 18-22 19-20 20-23 22-24 23-24

exact/norm bonds :

1-2 3-4 3-8 4-5 5-9 6-7 8-10 9-10 18-19 18-22 19-20 19-25 20-23 22-24
23-24 25-31 26-29 27-28

exact bonds :

1-14 1-15 2-3 4-16 5-6 7-13 17-18 17-27 20-21 21-26

G1:O,S,N,Se

Match level :

1:CLASS 2:CLASS 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom
21:CLASS 22:Atom 23:Atom 24:Atom 25:CLASS 26:CLASS 27:CLASS 28:Atom 29:Atom
31:Atom

Element Count :

Node 28: Limited
N,N1-2

Node 29: Limited
N,N1-2

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:01:27 FILE 'CASREACT'

SCREENING COMPLETE - 27 REACTIONS TO VERIFY FROM 3 DOCUMENTS

100.0% DONE 27 VERIFIED 0 HIT RXNS 0 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE** ✓
 BATCH **COMPLETE** ✓

PROJECTED VERIFICATIONS: 229 TO 851

PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1 (0 REACTIONS)

=> s l1 full ✓

FULL SEARCH INITIATED 16:01:35 FILE 'CASREACT'

SCREENING COMPLETE ✓ 192 REACTIONS TO VERIFY FROM 31 DOCUMENTS

100.0% DONE ✓ 192 VERIFIED 33 HIT RXNS ✓ 5 DOCS ✓

SEARCH TIME: 00.00.01

L3 5 SEA SSS FUL L1 (33 REACTIONS)

=> d ibib abs hit 1-5

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 145168977 CASREACT

TITLE:

Synthesis and spectroscopic characterization of heptamethine cyanine NIR dyes for their use in optochemical sensors
Encinas, Cristina; Miltsov, Serguei; Otazo, Elena; Rivera, Laia; Puyol, Mar; Alonso, Julian

AUTHOR(S):

CORPORATE SOURCE:

Autonomous University of Barcelona, Bellaterra,

08193,

SOURCE:

Spain
Dyes and Pigments (2005), Volume Date 2006, 71(1), 28-36

PUBLISHER:

CODEN: DYPIDX; ISSN: 0143-7208

DOCUMENT TYPE:

Elsevier Ltd.

LANGUAGE:

Journal

AB

A set of near-IR absorbing tricyanobocyanine dyes has been synthesized and characterized for their future application as chromolophores in optochem. sensors. Their absorption maxima are localized in the near-IR region, where matrix interferences are minimal and the use of suitable

and

inexpensive optical communication components gives great advantages. The acid form of the synthesized dyes in pure ethanol spans the region from 675 to 815 nm and the molar absorptivities are up to 3.3×10^5 L/mol cm. The calculated pKa values in ethanol lie between 11.4 and more than

13.

The effect of the introduction of substituents on the pKa values and on the spectroscopic characteristics of the dyes is also discussed.

Moreover, pH-sensitive aggregation processes have been observed in aqueous solution

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR

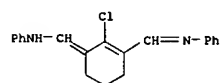
THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

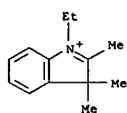
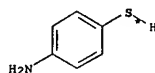
FORMAT

RX(15) OF 18 COMPOSED OF RX(1), RX(11)

RX(15) A + B + AA ==> AB



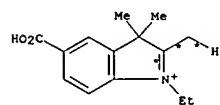
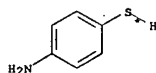
● HCl

● I⁻

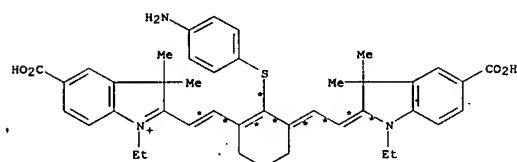
AA

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

● I⁻

AA

2
STEPS
→● I⁻

AC

YIELD 42%

RX(2) RCT A 63857-00-1, F 126442-85-1

RGT D 127-09-3 AcONa

PRO G 900807-92-3

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 30 minutes, reflux

SUBSTAGE(2) overnight, -10 deg C

NTE acid-base equilibrium studied

RX(12) RCT G 900807-92-3, AA 1193-02-8

PRO AC 900807-97-8

NTE no experimental detail, acid-base equilibrium studied

RX(18) OF 18 COMPOSED OF RX(7), RX(13)

RX(18) A + 2 P + AA ==> AD

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

2

STEPS
→

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(1) RCT A 63857-00-1, B 14134-81-7

RGT D 127-09-3 AcONa

PRO C 124591-86-2

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 30 minutes, reflux

SUBSTAGE(2) overnight, -10 deg C

NTE acid-base equilibrium studied

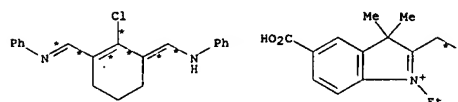
RX(11) RCT C 124591-86-2, AA 1193-02-8

PRO AB 264915-22-2

NTE no experimental detail, acid-base equilibrium studied

RX(16) OF 18 COMPOSED OF RX(2), RX(12)

RX(16) A + 2 F + AA ==> AC



● HCl

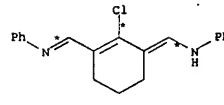
● I⁻

A

F

L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

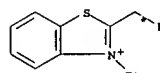
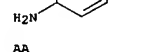


● HCl

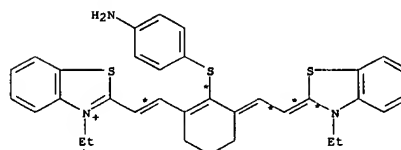
● I⁻

A

P

● I⁻

AA

2
STEPS
→● I⁻

AD

YIELD 45%

RX(7) RCT A 63857-00-1, P 31119-93-5

RGT D 127-09-3 AcONa

PRO Q 65303-15-3

SOL 64-17-5 EtOH

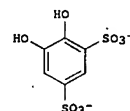
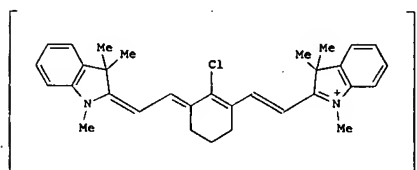
L3 ANSWER 1 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
 CON SUBSTAGE(1) 30 minutes, reflux
 SUBSTAGE(2) overnight, -10 deg C
 NTE acid-base equilibrium studied
 RX(13) RCT Q 65303-15-3, AA 1193-02-8
 PRO AD 900807-98-9
 NTE no experimental detail, acid-base equilibrium studied

L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 142:483447 CASREACT
 TITLE: Process for the preparation of infrared absorbing cyanine dyes with polysulfonate anions
 INVENTOR(S): Tao, Ting; Kottmair, Eduard; Beckley, Scott A.
 PATENT ASSIGNEE(S): USA
 SOURCE: U.S. Pat. Appl. Publ., 15 pp.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005113546	A1	20050526	US 2003-722257	20031125
US 7132550	B2	20061107		
EP 1535968	A2	20050601	EP 2004-27416	20041118
R: DE, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR, IS, YU			JP 2004-340997	20041125
JP 2005163039	A	20050623	US 2003-722257	20031125
PRIORITY APPLN. INFO.: GI				

Inventors

11/25/03

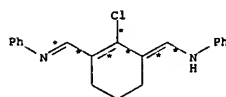


I

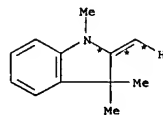
AB A convenient and economical method for preparing IR absorbing cyanine dyes

L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
 is useful in lithog. printing plate precursors is disclosed. The reaction
 generally carried out by condensation of a heterocyclic base contg. an
 activated methylene group and an unsatd. bisaldehyde or its equiv. in a
 solvent or solvent mixt. at about 20-150°. All the reactions
 necessary for prodn. of the IR absorbing cyanine dye may be carried out
 in one reaction vessel without isolating any intermediate products. Thus,
 2-chloro-1-formyl-3-hydroxymethylencyclohexene was reacted with
 1,3,3-trimethyl-2-methyleneindoline (Fisher's base) to give a dark-green
 soln. which was then added to a soln. contg. disodium 4,5-dihydroxy-1,3-
 benzenedisulfonate to give a ppt. of an IR absorbing cyanine dye (I).
 REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

RX(7) OF 14 ...G + 2 J + P + K ==> Q

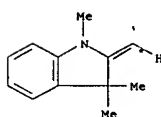


● HCl



G

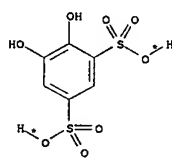
J



J



P

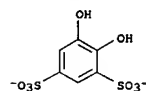


K

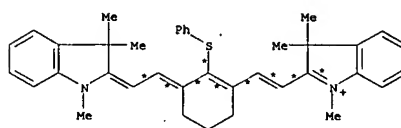
● 2 Na

(7) →

L3 ANSWER 2 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Q: CM 1



Q: CM 2

RX(7) RCT G 63857-00-1, J 118-12-7

STAGE(1)
 SOL 64-17-5 EtOH
 CON SUBSTAGE(1) 4 hours, 70 deg C
 SUBSTAGE(2) 70 deg C -> room temperature

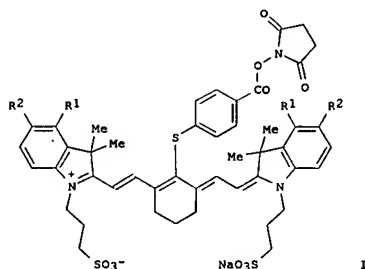
STAGE(2)
 RCT P 108-98-5
 RGT R 1310-73-2 NaOH
 SOL 64-17-5 EtOH
 CON 15 hours, room temperature

STAGE(3)
 RGT H 7647-01-0 HCl
 SOL 7732-18-5 Water
 CON 42 deg C

STAGE(4)
 RCT K 149-45-1
 SOL 7732-18-5 Water

PRO Q 491576-85-3

E3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 140:78500 CASREACT
 TITLE: Synthesis of water-soluble near-infrared cyanine dyes functionalized with [(succinimido)oxyl]carbonyl group
 AUTHOR(S): Strekowski, Lucjan; Mason, Christian J.; Lee, Hyeran; Gupta, Rajni; Sowell, John; Patonay, Gabor
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA
 SOURCE: Journal of Heterocyclic Chemistry (2003), 40(5), 913-916
 CODEN: JHCTAD; ISSN: 0022-152X
 PUBLISHER: HeteroCorporation
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Two heptamethine cyanine dyes I (R1 = R2 = H; R1R2 = (CH:CH)2) suitable for labeling of biomols. at a primary amino group with a near-IR chromophore/fluorophore ($\lambda_{max}/\lambda_{em}$ = 800/830 nm and 837/864 nm) have been synthesized from readily available starting materials. Despite the high mol. complexity of intermediate and final products, all these compds. have been obtained in an anal. pure form by using crystallization only.

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

RX(7) OF 13 COMPOSED OF RX(1), RX(3)
 RX(7) 2 A + B + G ==> K

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(1) RCT A 63666-10-4, B 63857-00-1
 RGT D 127-09-3 AcONa
 PRO C 640279-12-5
 SOL 64-17-5 EtOH
 NTE stereoselective

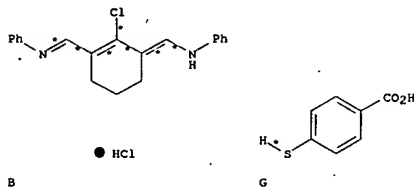
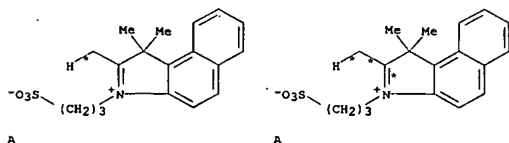
RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)
 SOL 68-12-2 DMF
 CON 24 hours, 23 deg C

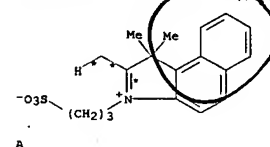
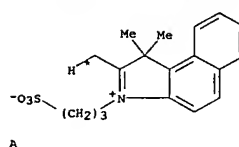
STAGE(2)
 SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

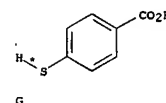
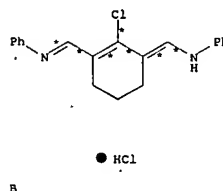
RX(11) OF 13 COMPOSED OF RX(1), RX(3), RX(5)
 RX(11) 2 A + B + G + L ==> N



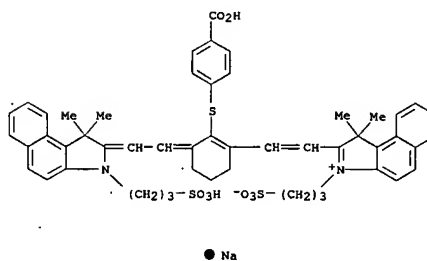
L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Not claimed

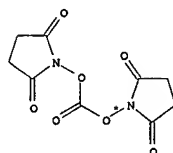


2 STEPS



K
 YIELD 90%

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



3 STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
 PAGE 2-A

N
 YIELD 88%

RX(1) RCT A 63666-10-4, B 63857-00-1
 RGT D 127-09-3 AcONa
 PRO C 640279-12-5
 SOL 64-17-5 EtOH
 NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)
 SOL 68-12-2 DMF
 CON 24 hours, 23 deg C

STAGE(2)
 SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

RX(5) RCT K 367251-79-4, L 74124-79-1

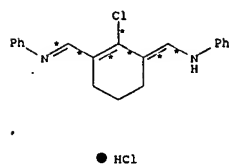
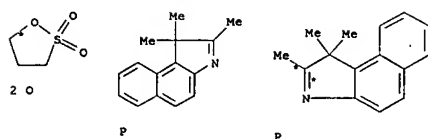
STAGE(1)
 SOL 68-12-2 DMF
 CON 24 hours, 23 deg C

STAGE(2)
 SOL 60-29-7 Et2O
 CON 30 minutes, 23 deg C

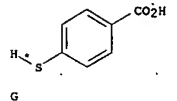
PRO N 367251-80-7

RX(12) OF 13 COMPOSED OF RX(6), RX(1), RX(3), RX(5)

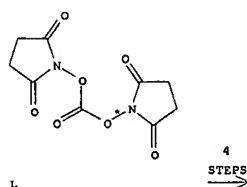
L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
RX(12) 2 O + 2 P + B + G + L ==> N



B



G

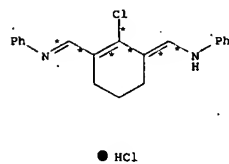
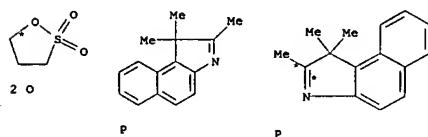


L

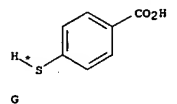
4
STEPS

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

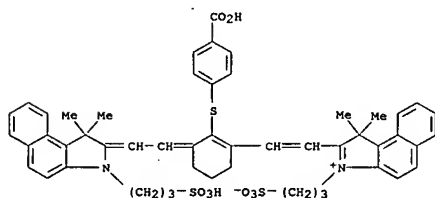


B



G

3
STEPS



K
YIELD 90%

RX(6) RCT O 1120-71-4, P 41532-84-7
PRO A 63666-10-4
NTE no exptl. detail

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

Na

N
YIELD 88%

RX(6) RCT O 1120-71-4, P 41532-84-7
PRO A 63666-10-4
NTE no exptl. detail

RX(1) RCT A 63666-10-4, B 63857-00-1
RGT D 127-09-3 AcONa
PRO C 640279-12-5
SOL 64-17-5 EtOH
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

STAGE(1)
SOL 68-12-2 DMF
CON 24 hours, 23 deg C

STAGE(2)
SOL 64-17-5 EtOH, 60-29-7 Et2O

PRO K 367251-79-4

RX(5) RCT K 367251-79-4, L 74124-79-1

STAGE(1)
SOL 68-12-2 DMF
CON 24 hours, 23 deg C

STAGE(2)
SOL 60-29-7 Et2O
CON 30 minutes, 23 deg C

PRO N 367251-80-7

RX(13) OF 13 COMPOSED OF RX(6), RX(1), RX(3)
RX(13) 2 O + 2 P + B + G ==> K

L3 ANSWER 3 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(1) RCT A 63666-10-4, B 63857-00-1
RGT D 127-09-3 AcONa
PRO C 640279-12-5
SOL 64-17-5 EtOH
NTE stereoselective

RX(3) RCT C 640279-12-5, G 1074-36-8

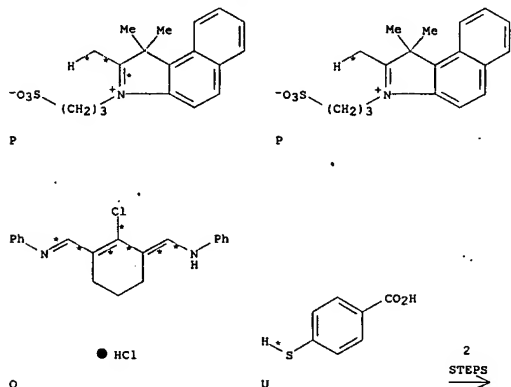
STAGE(1)
SOL 68-12-2 DMF
CON 24 hours, 23 deg C

STAGE(2)
SOL 64-17-5 EtOH, 60-29-7 Et2O

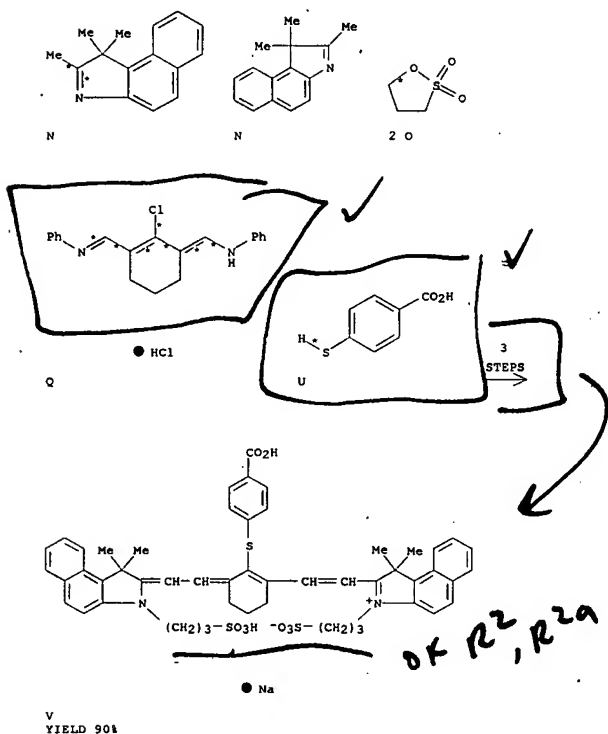
PRO K 367251-79-4

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 135:305176 CASREACT
 TITLE: New heptamethine cyanine reagents for labeling of biomolecules with a near-infrared chromophore
 AUTHOR(S): Strekowski, Lucjan; Gorecki, Tadeusz; Mason, J. Christian; Lee, Hyeran; Patonay, Gabor
 CORPORATE SOURCE: Department of Chemistry, Georgia State University, Atlanta, GA, 30303, USA
 SOURCE: Heterocyclic Communications (2001), 7(2), 117-122
 CODEN: HCOMEX; ISSN: 0793-0283
 PUBLISHER: Freund Publishing House Ltd.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The syntheses of two fluorescent cyanine dyes (λ_{max} = 1033 and 1060 nm in MeOH) with an isothiocyanato function and a succinimidoxycarbonyl-functionalized cyanine dye (λ_{max} = 837 nm in MeOH) for labeling of biomols. at amino groups are described.
 REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
 FORMAT

RX(10) OF 14 COMPOSED OF RX(5), RX(6)
 RX(10) 2 P + Q + U ==> V

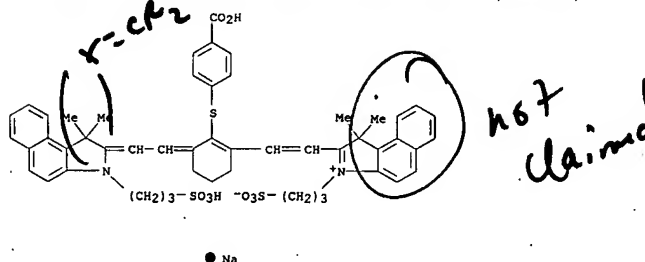


L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(4) RCT N 41532-84-7, O 1120-71-4
 PRO P 63666-10-4
 MTE literature prepn.

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



V
 YIELD 90%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)
 RGT S 127-09-3 AcONa
 SOL 64-17-5 EtOH

STAGE(2)
 SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)
 SOL 68-12-2 DMF

STAGE(2)
 SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(12) OF 14 COMPOSED OF RX(4), RX(5), RX(6)
 RX(12) 2 N + 2 O + Q + U ==> V

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)
 RGT S 127-09-3 AcONa
 SOL 64-17-5 EtOH

STAGE(2)
 SOL 60-29-7 Et2O

PRO R 259261-66-0

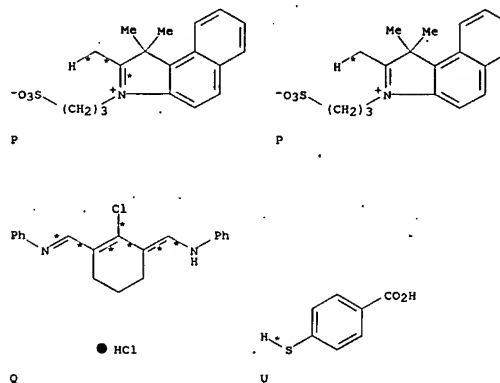
RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)
 SOL 68-12-2 DMF

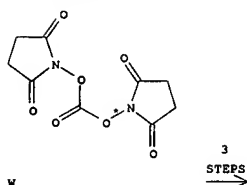
STAGE(2)
 SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(13) OF 14 COMPOSED OF RX(5), RX(6), RX(7)
 RX(13) 2 P + Q + U + W ==> X



L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

● Na

X
YIELD 91%

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)

RGT S 127-09-3 AcONa
SOL 64-17-5 EtOH

STAGE(2)

SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

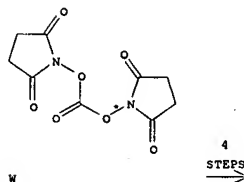
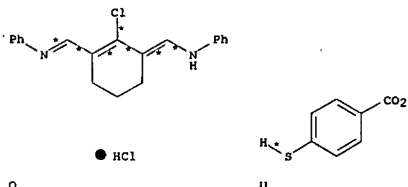
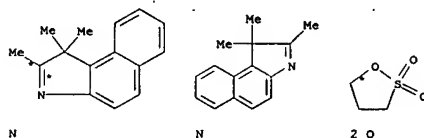
STAGE(1)

SOL 68-12-2 DMF

STAGE(2)

SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(7) RCT V 367251-79-4, W 74124-79-1
PRO X 367251-80-7
SOL 68-12-2 DMF
NTE literature prepn.L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
RX(14) OF 14 COMPOSED OF RX(4), RX(5), RX(6), RX(7)
RX(14) 2 N + 2 O + Q + U + W ==> X

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L3 ANSWER 4 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PAGE 2-A

● Na

X
YIELD 91%RX(4) RCT N 41532-84-7, O 1120-71-4
PRO P 63666-10-4
NTE literature prepn.

RX(5) RCT P 63666-10-4, Q 63857-00-1

STAGE(1)

RGT S 127-09-3 AcONa
SOL 64-17-5 EtOH

STAGE(2)

SOL 60-29-7 Et2O

PRO R 259261-66-0

RX(6) RCT R 259261-66-0, U 1074-36-8

STAGE(1)

SOL 68-12-2 DMF

STAGE(2)

SOL 60-29-7 Et2O

PRO V 367251-79-4

RX(7) RCT V 367251-79-4, W 74124-79-1
PRO X 367251-80-7
SOL 68-12-2 DMF
NTE literature prepn.

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 127:231448 CASREACT

TITLE: Functionalized Tricarbocyanine Dyes as Near-Infrared Fluorescent Probes for Biomolecules

AUTHOR(S): Flanagan, James H., Jr.; Khan, Shaheer H.; Menchen, Steve; Soper, Steven A.; Hammer, Robert P.

CORPORATE SOURCE: Department of Chemistry, Louisiana State University, Baton Rouge, LA, 70803-1804, USA

SOURCE: Bioconjugate Chemistry (1997), 8(5), 751-756

CODEN: BCCHEJ; ISSN: 1043-1802

PUBLISHER: American Chemical Society

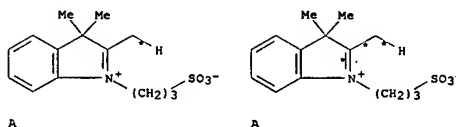
DOCUMENT TYPE: Journal

LANGUAGE: English

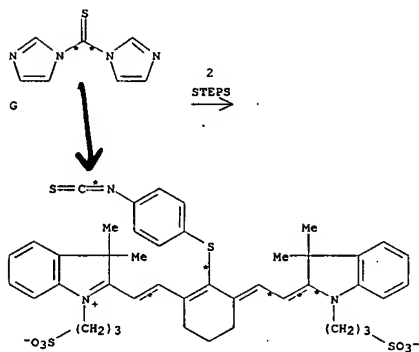
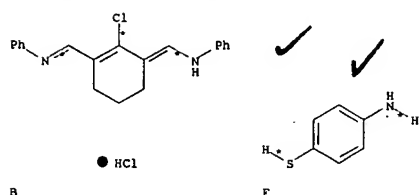
AB The syntheses of 3 novel functionalized tricarbocyanine dyes are described. These dyes containing isothiocyanate and succinimidyl ester functional groups are reactive toward primary amines and can be used as fluorescent probes for biol. pertinent compds. such as amino acids and functionalized dideoxynucleotides. The absorption and fluorescence maxima occur in the near-IR region of the spectrum (770-820 nm). The succinimidyl ester proved to be very sensitive to hydrolysis and was generated in situ to label amino acids and alkyl amines. The isothiocyanates were less susceptible to hydrolysis and were conjugated using organic modified [40% (volume/volume) acetonitrile] buffers to amino acids. A dye with an alkyl isothiocyanate moiety showed conjugation to amino-functionalized dideoxynucleotide triphosphates.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

RX(11) OF 44 COMPOSED OF RX(1), RX(2)
RX(11) 2 A + B + F + G ==> H

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

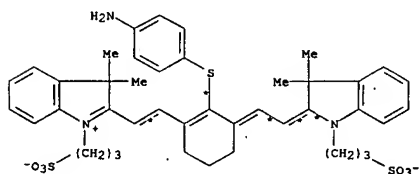


YIELD 29%

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



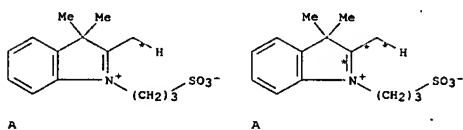
YIELD 50%

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)
 SOL 68-12-2 DMF
 STAGE(2)
 RCT C 160846-41-3
 PRO X 195382-11-7

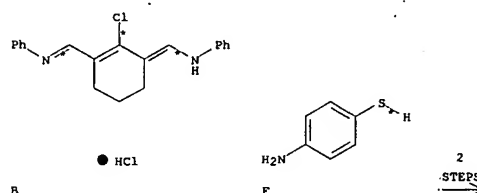
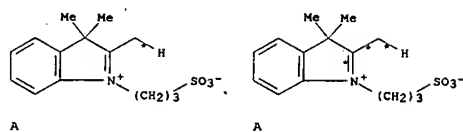
RX(13) OF 44 COMPOSED OF RX(1), RX(7)
 RX(13) 2 A + B + Y ==> Z



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

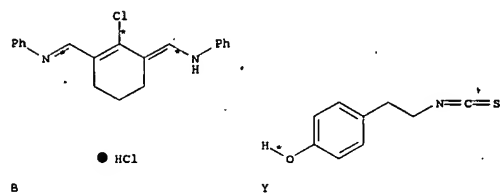
STAGE(1)
 SOL 68-12-2 DMF
 STAGE(2)
 RCT G 6160-65-2
 STAGE(3)
 SOL 60-29-7 Et2O
 STAGE(4)
 SOL 7732-18-5 Water, 67-56-1 MeOH
 PRO H 160846-42-4

RX(12) OF 44 COMPOSED OF RX(1), RX(6)
 RX(12) 2 A + B + F ==> X

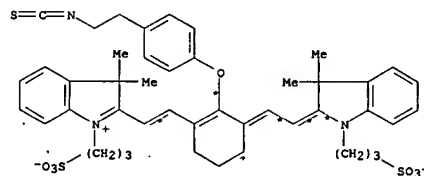


2 STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



2 STEPS



YIELD 32%

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7

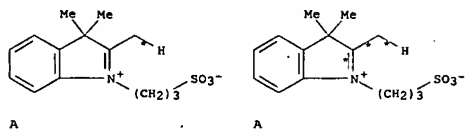
STAGE(1)
 RGT AA 7646-69-7 NaH
 SOL 68-12-2 DMF

STAGE(2)
 RCT C 160846-41-3
 SOL 68-12-2 DMF

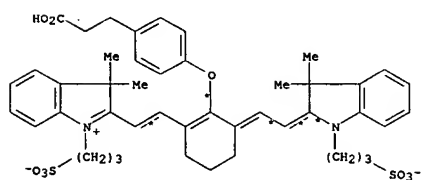
PRO Z 195382-08-2

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN
RX(14) OF 44 COMPOSED OF RX(1), RX(9)
RX(14) 2 A + B + AC ==> M

(Continued)



2
STEPS
→

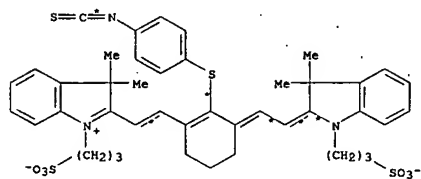


YIELD 31%

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)



YIELD 39%

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO X 195382-11-7

RX(10) RCT X 195382-11-7

STAGE(1)
RGT AE 497-19-8 Na2CO3
SOL 68-12-2 DMF

STAGE(2)
RCT AD 463-71-8

PRO H 160846-42-4

RX(21) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)
AND REACTION SEQUENCE RX(1), RX(7)
...AB + G ==> Y...
...2 A + B + Y ==> Z

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

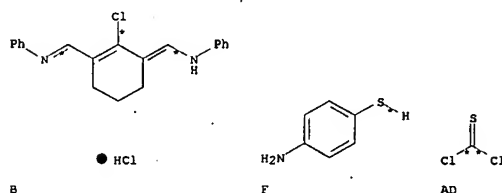
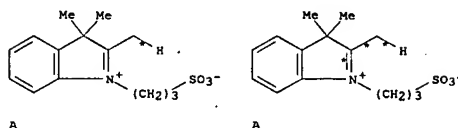
RX(9) RCT AC 501-97-3

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO M 195382-12-8

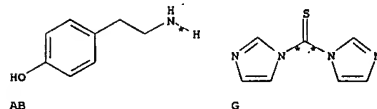
RX(20) OF 44 COMPOSED OF RX(1), RX(6), RX(10)
RX(20) 2 A + B + F + AD ==> H



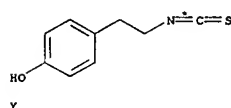
3
STEPS
→

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

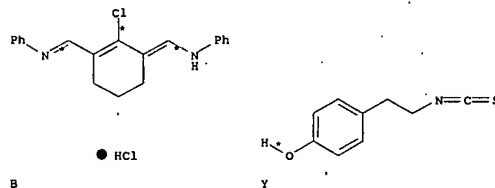
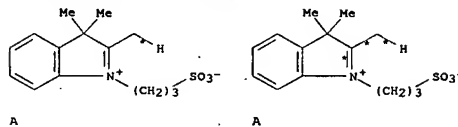
(Continued)



2
STEPS
→



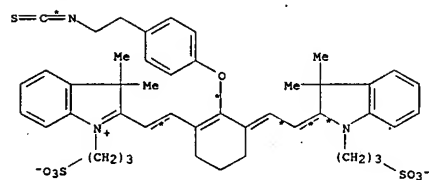
START NEXT REACTION SEQUENCE



2
STEPS
→

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

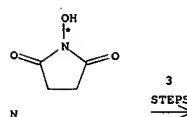
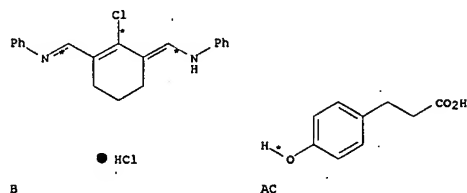
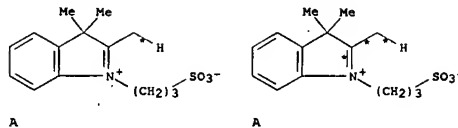


Z
YIELD 32%

RX(8) RCT AB 51-67-2
STAGE(1)
SOL 68-12-2 DMF
STAGE(2)
RCT G 6160-65-2
PRO Y 60114-04-7
RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH
RX(7) RCT Y 60114-04-7
STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF
STAGE(2)
RCT C 160846-41-3
SOL 68-12-2 DMF
PRO Z 195382-08-2

RX(22) OF 44 COMPOSED OF RX(1), RX(9), RX(3)
RX(22) 2 A + B + AC + N ==> O

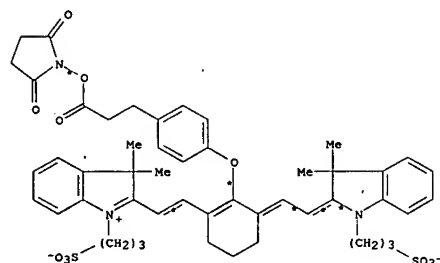
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



3
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN

(Continued)

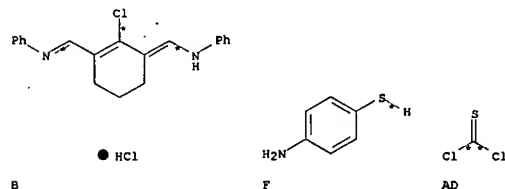
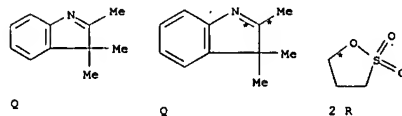


O

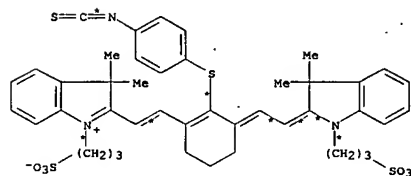
RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH
RX(9) RCT AC 501-97-3
STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF
STAGE(2)
RCT C 160846-41-3
PRO M 195382-12-8
RX(3) RCT M 195382-12-8, N 6066-82-6
STAGE(1)
SOL 68-12-2 DMF
STAGE(2)
RGT P 538-75-0 DCC
PRO O 195382-09-3

RX(23) OF 44 COMPOSED OF RX(4), RX(1), RX(6), RX(10)
RX(23) 2 Q + 2 R + B + F + AD ==> H

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



4
STEPS



H
YIELD 39%

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe
RX(1) RCT A 29636-96-2, B 195382-10-6

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

STAGE(1)
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO X 195382-11-7

RX(10) RCT X 195382-11-7

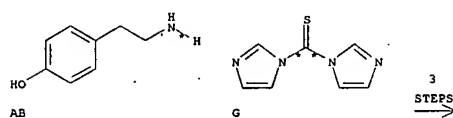
STAGE(1)
RGT AE 497-19-8 Na2CO3
SOL 68-12-2 DMF

STAGE(2)
RCT AD 463-71-8

PRO H 160846-42-4

RX(24) OF 44 COMPOSED OF REACTION SEQUENCE RX(8), RX(7)
AND REACTION SEQUENCE RX(4), RX(1), RX(7)

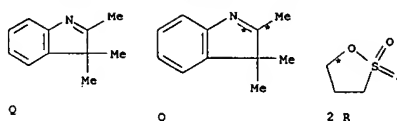
...AB + G ==> Y...
...2 Q + 2 R + B + Y ==> Z



START NEXT REACTION SEQUENCE

2

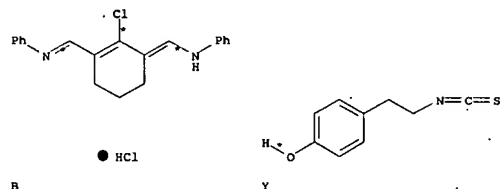
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Q

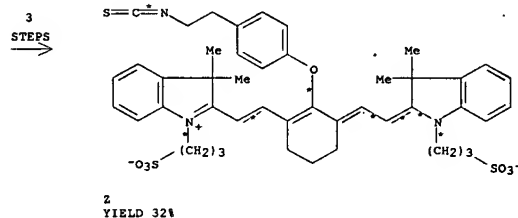
Q

2 R



B

Y



Z

YIELD 32%

RX(8) RCT AB 51-67-2

STAGE(1)
SOL 68-12-2 DMF

STAGE(2)
RCT G 6160-65-2

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

PRO Y 60114-04-7

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

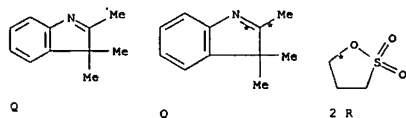
RX(7) RCT Y 60114-04-7

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3
SOL 68-12-2 DMF

PRO Z 195382-08-2

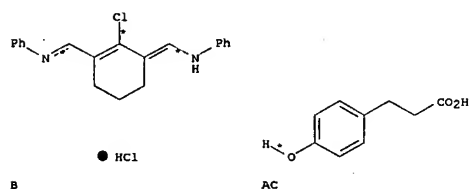
RX(25) OF 44 COMPOSED OF RX(4), RX(1), RX(9), RX(3)
RX(25) 2 Q + 2 R + B + AC + N ==> O



Q

Q

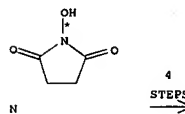
2 R



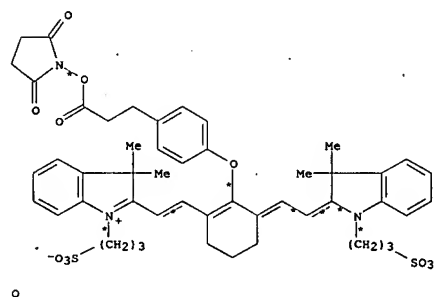
B

AC

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



N



O

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO M 195382-12-8

RX(3) RCT M 195382-12-8, N 6066-82-6

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

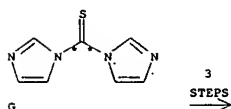
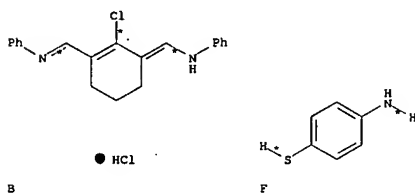
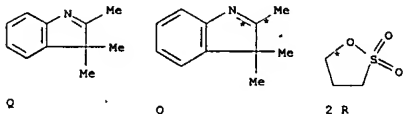
STAGE(1)

SOL 68-12-2 DMF

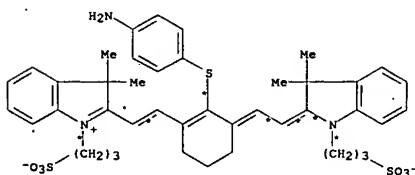
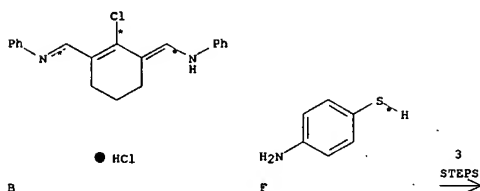
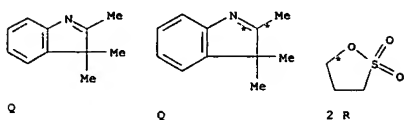
STAGE(2)

RGT P 538-75-0 DCC

PRO O 195382-09-3

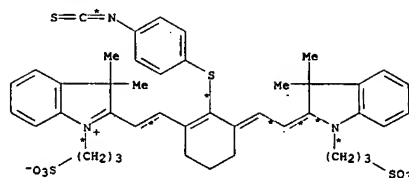
RX(29) OF 44 COMPOSED OF RX(4), RX(1), RX(2)
RX(29) 2 Q + 2 R + B + F + G ==> H

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

X
YIELD 50%RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMeRX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



YIELD 29%

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMeRX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)

SOL 68-12-2 DMF

STAGE(2)

RCT G 6160-65-2

STAGE(3)

SOL 60-29-7 Et2O

STAGE(4)

SOL 7732-18-5 Water, 67-56-1 MeOH

PRO H 160846-42-4

RX(30) OF 44 COMPOSED OF RX(4), RX(1), RX(6)
RX(30) 2 Q + 2 R + B + F ==> X

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

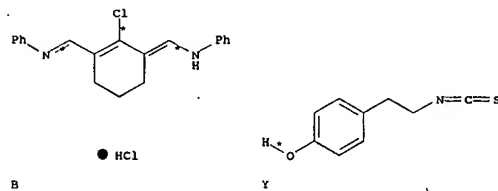
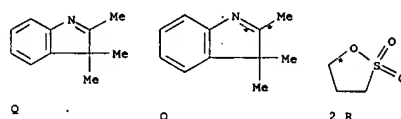
STAGE(1)

SOL 68-12-2 DMF

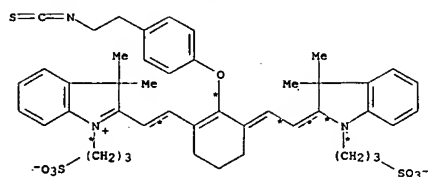
STAGE(2)

RCT C 160846-41-3

PRO X 195382-11-7

RX(31) OF 44 COMPOSED OF RX(4), RX(1), RX(7)
RX(31) 2 Q + 2 R + B + Y ==> Z3
STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

Z
YIELD 32%

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

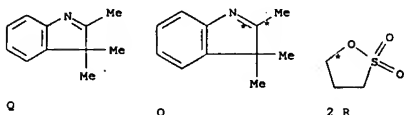
RX(7) RCT Y 60114-04-7

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3
SOL 68-12-2 DMF

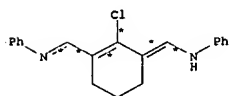
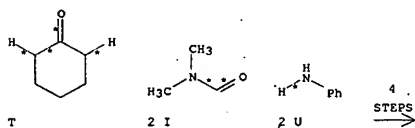
PRO Z 195382-08-2

RX(32) OF 44 COMPOSED OF RX(4), RX(1), RX(9)
RX(32) 2 Q + 2 R + B + AC ==> M



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

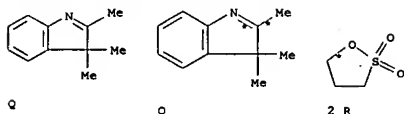
RX(38) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(6), RX(10)
AND REACTION SEQUENCE RX(4), RX(1), RX(6), RX(10)
...T + 2 I + 2 U ==> B...
...2 Q + 2 R + B + F + AD ==> H



● HCl

B

START NEXT REACTION SEQUENCE

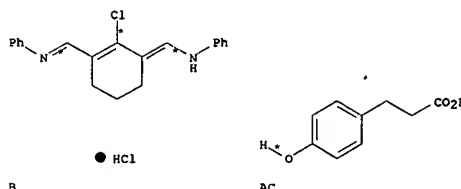


Q

Q

2 R

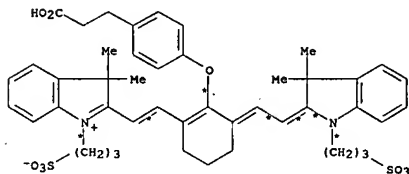
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



B

● HCl

AC

3
STEPSM
YIELD 31%

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

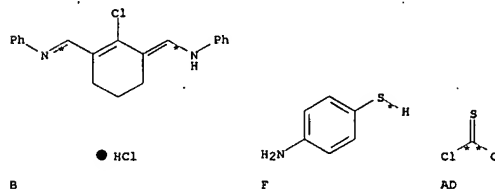
RX(9) RCT AC 501-97-3

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO M 195382-12-8

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

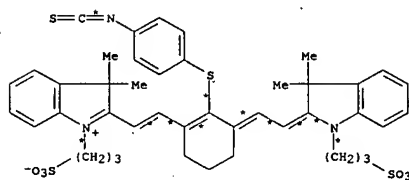


B

● HCl

F

AD

4
STEPSH
YIELD 39%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)
RGT V 10025-87-3 POCl3
SOL 68-12-2 DMF

STAGE(2)
RCT U 62-53-3
SOL 64-17-5 EtOH

STAGE(3)
RGT W 7647-01-0 HCl
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4

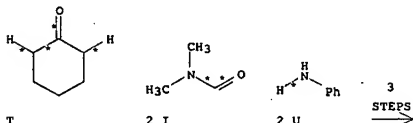
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
 PRO A 29636-96-2
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8
 STAGE(1)
 SOL 68-12-2 DMF
 STAGE(2)
 RCT C 160846-41-3
 PRO X 195382-11-7

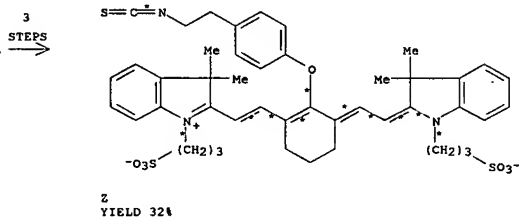
RX(10) RCT X 195382-11-7
 STAGE(1)
 RGT AE 497-19-8 Na2CO3
 SOL 68-12-2 DMF
 STAGE(2)
 RCT AD 463-71-8
 PRO H 160846-42-4

RX(39) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(7)
 AND REACTION SEQUENCE RX(8), RX(7)
 AND REACTION SEQUENCE RX(4), RX(1), RX(7)
 ...T + 2 I + 2 U ==> B...
 ...AB + G ==> Y...
 ...2 Q + 2 R + B + Y ==> Z



START NEXT REACTION SEQUENCE

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



RX(5) RCT T 108-94-1, I 68-12-2
 STAGE(1)
 RGT V 10025-87-3 POCl3
 SOL 68-12-2 DMF

STAGE(2)
 RCT U 62-53-3
 SOL 64-17-5 EtOH

STAGE(3)
 RGT W 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(8) RCT AB 51-67-2
 STAGE(1)
 SOL 68-12-2 DMF
 STAGE(2)
 RCT G 6160-65-2

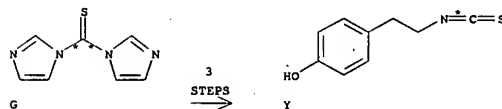
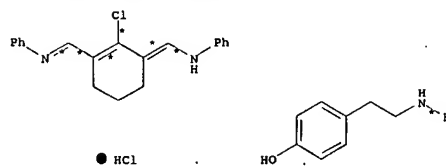
PRO Y 60114-04-7

RX(4) RCT Q 1640-39-7, R 1120-71-4
 PRO A 29636-96-2
 SOL 108-88-3 PhMe

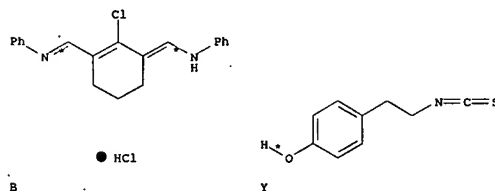
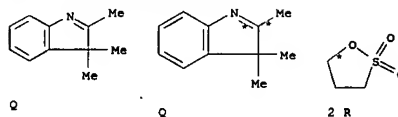
RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7
 STAGE(1)
 RGT AA 7646-69-7 NaH

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



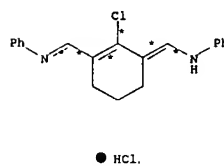
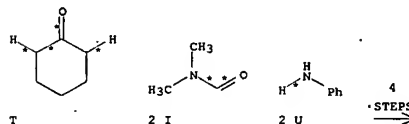
START NEXT REACTION SEQUENCE



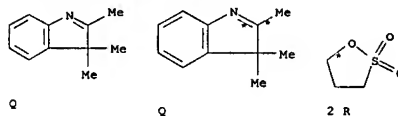
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)
 RCT C 160846-41-3
 SOL 68-12-2 DMF
 PRO Z 195382-08-2

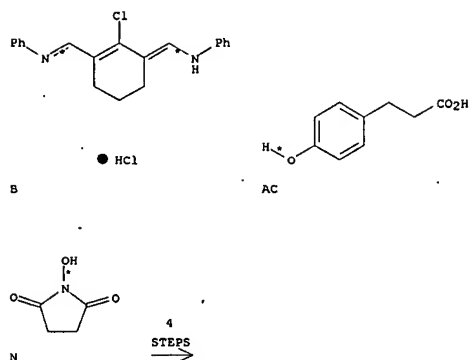
RX(40) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(9), RX(3)
 AND REACTION SEQUENCE RX(4), RX(1), RX(9), RX(3)
 ...T + 2 I + 2 U ==> B...
 ...2 Q + 2 R + B + AC + N ==> O



START NEXT REACTION SEQUENCE



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)
RGT V 10025-87-3 POC13
SOL 68-12-2 DMF

STAGE(2)
RCT U 62-53-3
SOL 64-17-5 EtOH

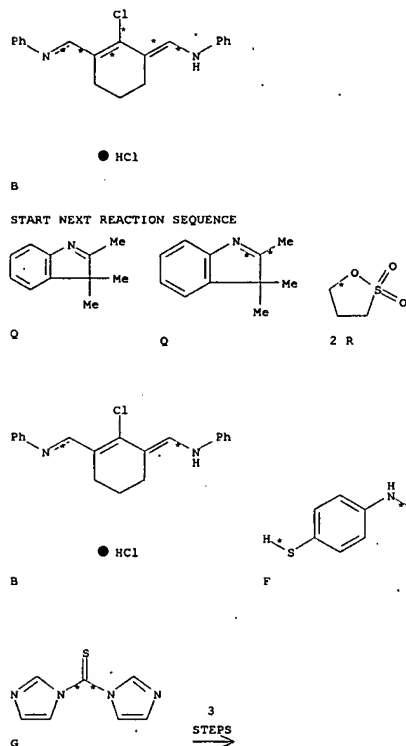
STAGE(3)
RGT W 7647-01-0 HCl
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

SOL 64-17-5 EtOH
RX(9) RCT AC 501-97-3

STAGE(1)
RGT AA 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)
RCT C 160846-41-3

PRO M 195382-12-8

RX(3) RCT M 195382-12-8, N 6066-82-6

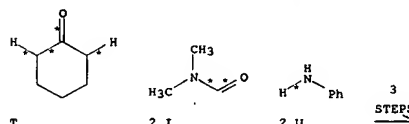
STAGE(1)
SOL 68-12-2 DMF

STAGE(2)
RGT P 538-75-0 DCC

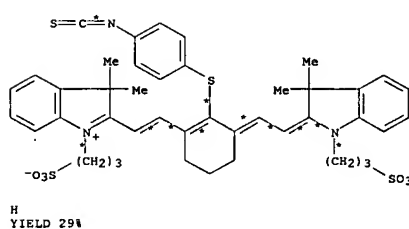
PRO O 195382-09-3

RX(41) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(2)
AND REACTION SEQUENCE RX(4), RX(1), RX(2)

...T + 2 I + 2 U ==> B...
...2 Q + 2 R + B + F + G ==> H



L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

H
YIELD 29%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)
RGT V 10025-87-3 POC13
SOL 68-12-2 DMF

STAGE(2)
RCT U 62-53-3
SOL 64-17-5 EtOH

STAGE(3)
RGT W 7647-01-0 HCl
SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4
PRO A 29636-96-2
SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
RGT D 127-09-3 AcONa
PRO C 160846-41-3
SOL 64-17-5 EtOH

RX(2) RCT F 1193-02-8, C 160846-41-3

STAGE(1)
SOL 68-12-2 DMF

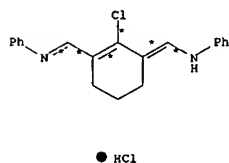
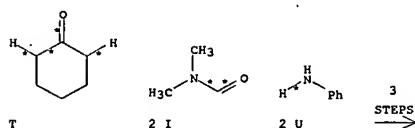
STAGE(2)
RCT G 6160-65-2

STAGE(3)
SOL 60-29-7 Et2O

STAGE(4)
SOL 7732-18-5 Water, 67-56-1 MeOH

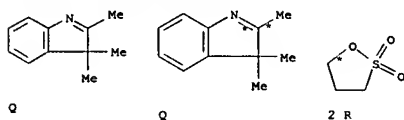
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)
PRO H 160846-42-4

RX(42) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(6)
AND REACTION SEQUENCE RX(4), RX(1), RX(6)
...T + 2 I + 2 U ==> B...
...2 Q + 2 R + B + F ==> X



B

START NEXT REACTION SEQUENCE



Q

Q

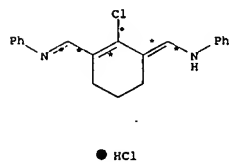
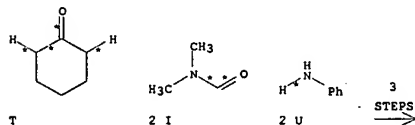
2 R

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(6) RCT F 1193-02-8
 STAGE(1)
 SOL 68-12-2 DMF
 STAGE(2)
 RCT C 160846-41-3
 PRO X 195382-11-7

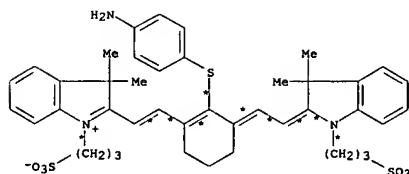
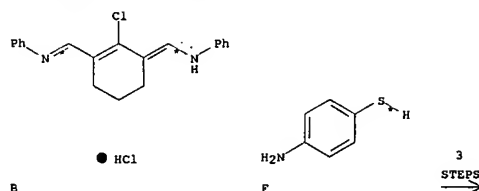
RX(43) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(7)
AND REACTION SEQUENCE RX(4), RX(1), RX(7)
...T + 2 I + 2 U ==> B...
...2 Q + 2 R + B + Y ==> Z



B

START NEXT REACTION SEQUENCE

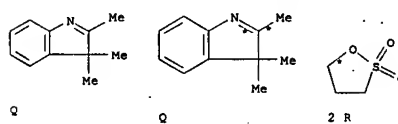
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



X
YIELD 50%

RX(5) RCT T 108-94-1, I 68-12-2
 STAGE(1)
 RGT V 10025-87-3 POC13
 SOL 68-12-2 DMF
 STAGE(2)
 RCT U 62-53-3
 SOL 64-17-5 EtOH
 STAGE(3)
 RGT W 7647-01-0 HCl
 SOL 7732-18-5 Water
 PRO B 195382-10-6
RX(4) RCT Q 1640-39-7, R 1120-71-4
 PRO A 29636-96-2
 SOL 108-88-3 PhMe

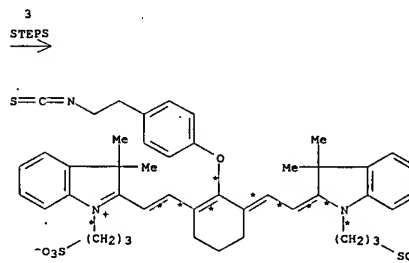
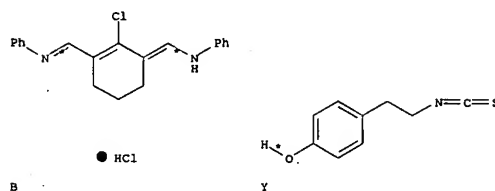
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



Q

Q

2 R



Z
YIELD 32%

RX(5) RCT T 108-94-1, I 68-12-2
 STAGE(1)
 RGT V 10025-87-3 POC13
 SOL 68-12-2 DMF

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)

STAGE(2)
 RCT U 62-53-3
 SOL 64-17-5 EtOH

STAGE(3)
 RGT W 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4
 PRO A 29636-96-2
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(7) RCT Y 60114-04-7

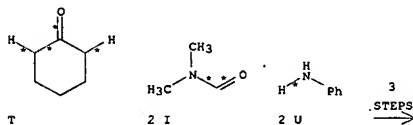
STAGE(1)
 RGT AA 7646-69-7 NaH
 SOL 68-12-2 DMF

STAGE(2)
 RCT C 160846-41-3
 SOL 68-12-2 DMF

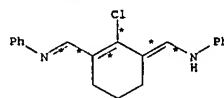
PRO Z 195382-08-2

RX(44) OF 44 COMPOSED OF REACTION SEQUENCE RX(5), RX(1), RX(9)
 AND REACTION SEQUENCE RX(4), RX(1), RX(9)

...T + 2 I + 2 U ==> B...
 ...2 Q + 2 R + B + AC ==> H



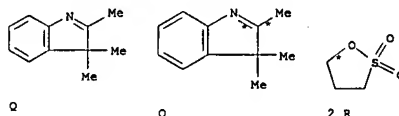
L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



● HCl

B

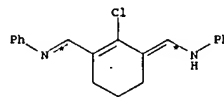
START NEXT REACTION SEQUENCE



Q

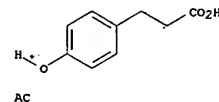
Q

2 R



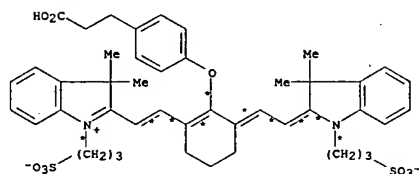
● HCl

B



3 STEPS

L3 ANSWER 5 OF 5 CASREACT COPYRIGHT 2007 ACS on STN (Continued)



M
 YIELD 31%

RX(5) RCT T 108-94-1, I 68-12-2

STAGE(1)
 RGT V 10025-87-3 POCl3
 SOL 68-12-2 DMF

STAGE(2)
 RCT U 62-53-3
 SOL 64-17-5 EtOH

STAGE(3)
 RGT W 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO B 195382-10-6

RX(4) RCT Q 1640-39-7, R 1120-71-4
 PRO A 29636-96-2
 SOL 108-88-3 PhMe

RX(1) RCT A 29636-96-2, B 195382-10-6
 RGT D 127-09-3 AcONa
 PRO C 160846-41-3
 SOL 64-17-5 EtOH

RX(9) RCT AC 501-97-3

STAGE(1)
 RGT AA 7646-69-7 NaH
 SOL 68-12-2 DMF

STAGE(2)
 RCT C 160846-41-3

PRO M 195382-12-8